



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 03:25 pm BST

PDB ID : 4FSL
Title : Crystal structure of beta-site app-cleaving enzyme 1 (BACE-DB-MUT) complex with N-(N-(4- acetamido-3-chloro-5-methylbenzyl)carbamidoyl)-3-(4-methoxyphenyl)-5-methyl-4-isothiazolecarboxamide
Authors : Muckelbauer, J.K.
Deposited on : 2012-06-27
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

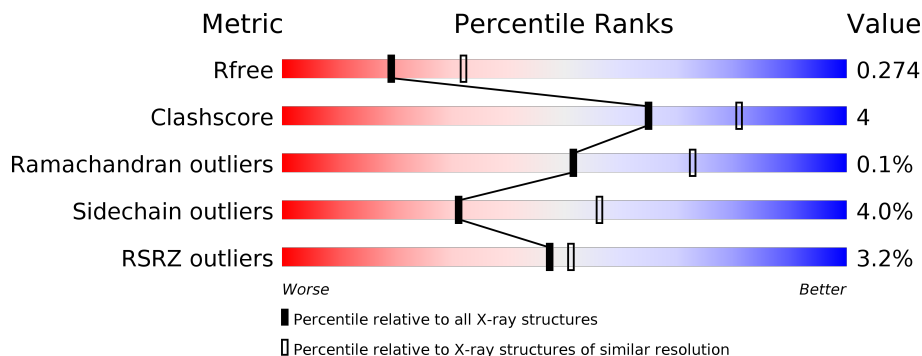
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	412	
1	B	412	
1	D	412	
1	E	412	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	0VB	A	501	-	X	-	-
2	0VB	B	501	-	X	-	-
2	0VB	D	501	-	X	-	-
2	0VB	E	501	-	X	-	-
3	IOD	A	502	-	-	X	-
3	IOD	B	503	-	-	X	-
3	IOD	D	502	-	-	X	-
3	IOD	E	502	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 13119 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

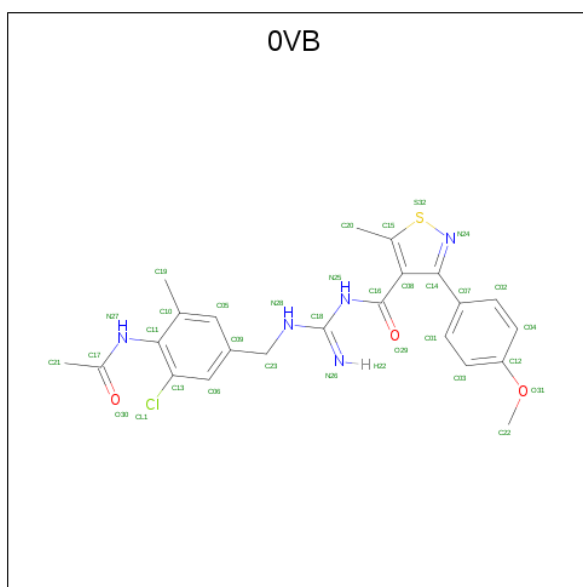
- Molecule 1 is a protein called Beta-secretase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	387	3036	1943	504	575	14	0	0	0
1	B	387	3038	1945	505	574	14	0	0	0
1	D	387	3042	1948	505	575	14	0	0	0
1	E	387	3040	1946	505	575	14	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	43	LYS	ARG	CONFLICT	UNP P56817
A	44	LYS	ARG	CONFLICT	UNP P56817
A	441	THR	-	EXPRESSION TAG	UNP P56817
B	43	LYS	ARG	CONFLICT	UNP P56817
B	44	LYS	ARG	CONFLICT	UNP P56817
B	441	THR	-	EXPRESSION TAG	UNP P56817
D	43	LYS	ARG	CONFLICT	UNP P56817
D	44	LYS	ARG	CONFLICT	UNP P56817
D	441	THR	-	EXPRESSION TAG	UNP P56817
E	43	LYS	ARG	CONFLICT	UNP P56817
E	44	LYS	ARG	CONFLICT	UNP P56817
E	441	THR	-	EXPRESSION TAG	UNP P56817

- Molecule 2 is N-{N-[4-(acetylamino)-3-chloro-5-methylbenzyl]carbamimidoyl}-3-(4-methoxyphenyl)-5-methyl-1,2-thiazole-4-carboxamide (three-letter code: 0VB) (formula: C₂₃H₂₄ClN₅O₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	Cl	N	O			S
2	A	1	Total 33	C 23	Cl 1	N 5	O 3	S 1	0	0
2	B	1	Total 33	C 23	Cl 1	N 5	O 3	S 1	0	0
2	D	1	Total 33	C 23	Cl 1	N 5	O 3	S 1	0	0
2	E	1	Total 33	C 23	Cl 1	N 5	O 3	S 1	0	0

- Molecule 3 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	3	Total 3 I 3	0	0
3	A	3	Total 3 I 3	0	0
3	D	3	Total 3 I 3	0	0
3	E	3	Total 3 I 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	215	Total 215 O 215	0	0

Continued on next page...

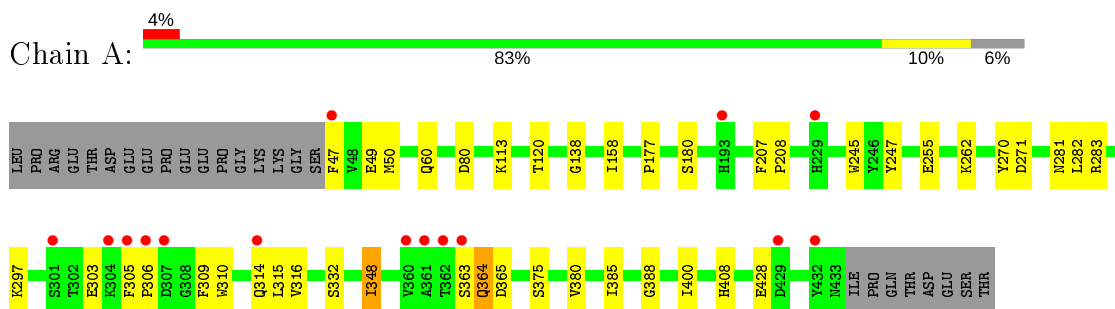
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	211	Total 211	O 211	0	0
4	D	182	Total 182	O 182	0	0
4	E	211	Total 211	O 211	0	0

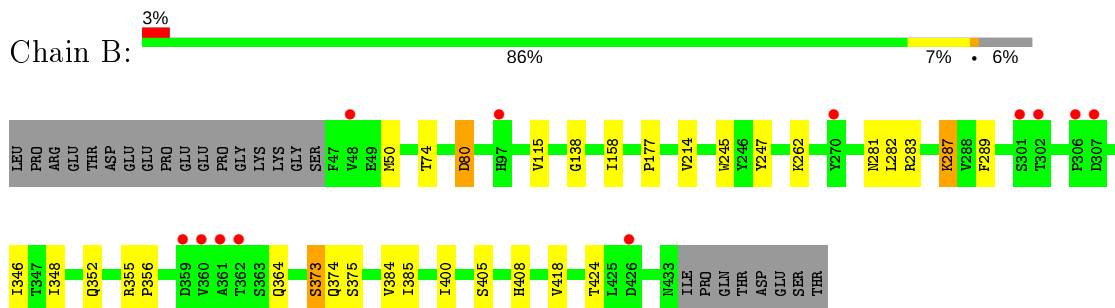
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

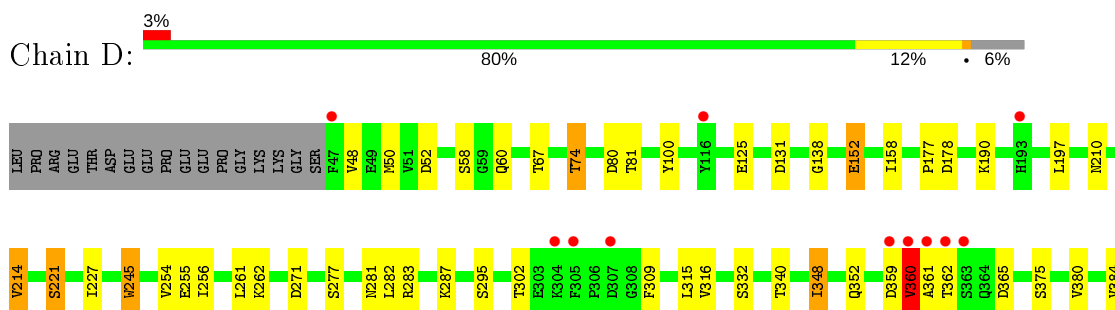
- Molecule 1: Beta-secretase 1



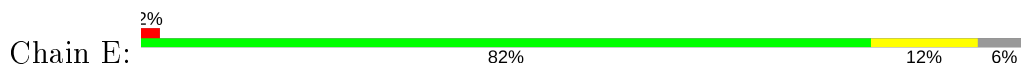
- Molecule 1: Beta-secretase 1

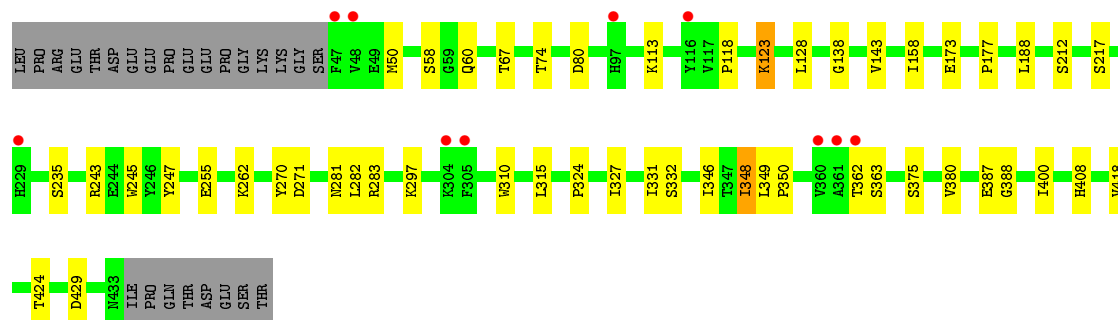


- Molecule 1: Beta-secretase 1



- Molecule 1: Beta-secretase 1





4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	86.54Å 131.18Å 90.31Å 90.00° 97.61° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 39.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.5 (50.00-2.50) 96.6 (39.00-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.48 (at 2.51Å)	Xtrriage
Refinement program	REFMAC 5.2.0019, CNS	Depositor
R, R_{free}	0.224 , 0.277 0.223 , 0.274	Depositor DCC
R_{free} test set	3377 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	30.1	Xtrriage
Anisotropy	0.071	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtrriage
Estimated twinning fraction	0.003 for l,-k,h	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13119	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.87 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.4340e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: IOD, 0VB

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.36	0/3114	0.52	0/4236
1	B	0.40	2/3116 (0.1%)	0.57	2/4237 (0.0%)
1	D	0.37	0/3120	0.53	0/4243
1	E	0.36	0/3118	0.52	0/4240
All	All	0.37	2/12468 (0.0%)	0.53	2/16956 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	80	ASP	CG-OD2	7.20	1.42	1.25
1	B	80	ASP	CB-CG	-5.01	1.41	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	80	ASP	CB-CG-OD1	12.36	129.42	118.30
1	B	80	ASP	CB-CG-OD2	-7.64	111.42	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3036	0	2933	25	0
1	B	3038	0	2939	17	0
1	D	3042	0	2953	30	0
1	E	3040	0	2944	26	0
2	A	33	0	24	4	0
2	B	33	0	24	3	0
2	D	33	0	24	2	0
2	E	33	0	24	4	0
3	A	3	0	0	2	0
3	B	3	0	0	3	0
3	D	3	0	0	3	0
3	E	3	0	0	3	0
4	A	215	0	0	5	0
4	B	211	0	0	3	0
4	D	182	0	0	2	0
4	E	211	0	0	1	0
All	All	13119	0	11865	99	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (99) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:118:PRO:HA	1:E:123:LYS:HB3	1.56	0.86
1:A:363:SER:HB3	4:A:667:HOH:O	1.75	0.85
1:E:173:GLU:OE2	1:E:243:ARG:NH1	2.21	0.74
1:D:359:ASP:OD2	1:D:360:VAL:HG13	1.90	0.72
1:A:365:ASP:HB2	4:A:667:HOH:O	1.93	0.68
1:A:262:LYS:HE2	4:B:625:HOH:O	2.02	0.58
1:E:177:PRO:HB3	3:E:503:IOD:I	2.73	0.58
1:D:81:THR:H	1:D:277:SER:HB2	1.68	0.58
1:A:305:PHE:HD2	1:A:316:VAL:HG21	1.68	0.58
2:A:501:0VB:H18	3:A:502:IOD:I	2.74	0.57
1:B:289:PHE:CD2	1:B:374:GLN:HB3	2.40	0.56
1:D:360:VAL:HG22	1:D:361:ALA:N	2.21	0.55
1:A:309:PHE:CD1	1:A:316:VAL:HG23	2.41	0.55
1:D:283:ARG:HB3	1:D:375:SER:HB2	1.89	0.55
1:E:283:ARG:HB2	1:E:380:VAL:HB	1.89	0.54
1:A:283:ARG:HB3	1:A:375:SER:HB2	1.89	0.54
1:B:283:ARG:HB3	1:B:375:SER:HB2	1.90	0.54
1:A:158:ILE:HG12	2:A:501:0VB:H15	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:67:THR:HG22	1:E:74:THR:HG22	1.90	0.54
1:D:255:GLU:HB2	1:D:332:SER:HB2	1.89	0.53
1:B:287:LYS:HD2	4:B:615:HOH:O	2.07	0.53
1:E:283:ARG:HB3	1:E:375:SER:HB2	1.90	0.53
1:A:283:ARG:HB2	1:A:380:VAL:HB	1.92	0.52
1:A:80:ASP:OD2	2:A:501:0VB:N26	2.38	0.52
1:D:256:ILE:HG12	1:D:261:LEU:HD21	1.92	0.52
1:B:346:ILE:HG22	1:B:418:VAL:HG22	1.92	0.51
1:E:113:LYS:HD2	1:E:128:LEU:HD12	1.92	0.51
1:A:49:GLU:HG2	1:A:50:MET:HG3	1.93	0.50
1:E:80:ASP:OD1	2:E:501:0VB:N26	2.44	0.50
1:D:210:ASN:O	1:D:214:VAL:HG22	2.12	0.49
1:E:158:ILE:HG12	2:E:501:0VB:H15	1.93	0.49
1:D:80:ASP:HA	1:D:277:SER:HB2	1.94	0.49
1:A:60:GLN:HG3	4:A:642:HOH:O	2.12	0.49
1:B:373:SER:HB3	4:B:676:HOH:O	2.12	0.49
1:E:297:LYS:HG2	1:E:310:TRP:CZ2	2.47	0.49
1:D:227:ILE:HG23	1:D:390:TYR:HE2	1.78	0.49
1:D:359:ASP:OD1	1:D:365:ASP:HB2	2.13	0.48
1:A:247:TYR:HB3	1:A:400:ILE:HD11	1.95	0.48
1:A:80:ASP:OD1	2:A:501:0VB:N26	2.46	0.48
1:D:281:ASN:HB2	3:D:502:IOD:I	2.84	0.48
1:D:80:ASP:OD1	2:D:501:0VB:N26	2.47	0.47
1:D:125:GLU:HG2	1:D:152:GLU:HB3	1.96	0.47
1:D:352:GLN:O	1:D:384:VAL:HB	2.14	0.47
1:E:283:ARG:NH2	3:E:502:IOD:I	3.17	0.47
1:B:158:ILE:HG12	2:B:501:0VB:H15	1.96	0.47
1:D:254:VAL:HG12	1:D:261:LEU:HD23	1.97	0.46
1:A:255:GLU:HB2	1:A:332:SER:HB2	1.97	0.46
1:A:306:PRO:HB2	1:A:314:GLN:OE1	2.16	0.46
1:A:50:MET:HG2	1:A:138:GLY:HA2	1.96	0.46
1:B:80:ASP:OD2	2:B:501:0VB:N26	2.46	0.45
1:E:388:GLY:HA2	1:E:408:HIS:HB2	1.97	0.45
1:D:158:ILE:HG12	2:D:501:0VB:H15	1.98	0.45
1:A:364:GLN:HB2	4:A:815:HOH:O	2.17	0.45
1:E:363:SER:HB2	4:E:765:HOH:O	2.17	0.45
1:A:388:GLY:HA2	1:A:408:HIS:HB2	1.97	0.45
1:B:355:ARG:HA	1:B:356:PRO:HD3	1.85	0.45
1:B:80:ASP:OD1	2:B:501:0VB:N26	2.49	0.45
1:D:309:PHE:CD1	1:D:316:VAL:HG23	2.52	0.45
1:A:281:ASN:HB2	3:A:502:IOD:I	2.87	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:80:ASP:CG	2:E:501:0VB:H22	2.20	0.44
1:A:297:LYS:HE2	1:A:310:TRP:CD1	2.53	0.44
1:B:247:TYR:HB3	1:B:400:ILE:HD11	2.00	0.43
1:B:348:ILE:HD13	1:B:385:ILE:CD1	2.49	0.43
1:D:58:SER:HB3	1:D:387:GLU:OE1	2.18	0.43
1:D:74:THR:HG23	4:D:774:HOH:O	2.19	0.43
1:E:270:TYR:HA	1:E:271:ASP:HA	1.69	0.43
1:E:281:ASN:HB2	3:E:502:IOD:I	2.88	0.43
1:D:52:ASP:H	1:D:221:SER:HB3	1.82	0.43
1:E:331:ILE:HB	1:E:348:ILE:HG12	2.00	0.43
1:A:270:TYR:HA	1:A:271:ASP:HA	1.70	0.43
1:E:58:SER:HB3	1:E:387:GLU:OE1	2.19	0.43
1:B:352:GLN:O	1:B:384:VAL:HB	2.19	0.43
1:D:50:MET:HG2	1:D:138:GLY:HA2	2.00	0.43
1:D:177:PRO:HB3	3:D:503:IOD:I	2.89	0.42
1:E:143:VAL:HG11	1:E:188:LEU:HA	2.00	0.42
1:E:247:TYR:HB3	1:E:400:ILE:HD11	2.00	0.42
1:D:190:LYS:HE3	1:D:190:LYS:HB2	1.85	0.42
1:D:348:ILE:HG22	4:D:777:HOH:O	2.19	0.42
1:D:256:ILE:HG21	1:D:295:SER:HB3	2.00	0.42
1:E:349:LEU:HB3	1:E:350:PRO:HD2	2.01	0.42
1:A:207:PHE:HB2	1:A:208:PRO:HD2	2.02	0.42
1:B:281:ASN:HB2	3:B:502:IOD:I	2.90	0.42
1:D:245:TRP:CD1	1:D:245:TRP:N	2.87	0.42
1:E:255:GLU:HB2	1:E:332:SER:HB2	2.01	0.42
1:A:113:LYS:HE3	1:A:177:PRO:HG2	2.02	0.41
1:B:177:PRO:HB3	3:B:503:IOD:I	2.90	0.41
1:E:80:ASP:CG	2:E:501:0VB:N26	2.74	0.41
1:E:50:MET:HG2	1:E:138:GLY:HA2	2.03	0.41
1:D:100:TYR:OH	1:D:131:ASP:OD2	2.37	0.41
1:D:283:ARG:HB2	1:D:380:VAL:HB	2.02	0.41
1:A:47:PHE:N	4:A:765:HOH:O	2.53	0.41
1:B:405:SER:HB3	1:B:408:HIS:HB3	2.01	0.41
1:E:324:PRO:O	1:E:327:ILE:HG12	2.20	0.41
1:A:348:ILE:HD13	1:A:385:ILE:HD12	2.03	0.41
1:B:115:VAL:HA	3:B:503:IOD:I	2.91	0.41
1:B:50:MET:HG2	1:B:138:GLY:HA2	2.03	0.40
1:D:283:ARG:NH2	3:D:502:IOD:I	3.24	0.40
1:D:408:HIS:CE1	1:D:415:THR:OG1	2.75	0.40
1:E:346:ILE:HG22	1:E:418:VAL:HG22	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	385/412 (93%)	378 (98%)	7 (2%)	0	100	100
1	B	385/412 (93%)	374 (97%)	11 (3%)	0	100	100
1	D	385/412 (93%)	375 (97%)	9 (2%)	1 (0%)	41	61
1	E	385/412 (93%)	377 (98%)	8 (2%)	0	100	100
All	All	1540/1648 (93%)	1504 (98%)	35 (2%)	1 (0%)	51	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	360	VAL

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	328/353 (93%)	319 (97%)	9 (3%)	44	71
1	B	328/353 (93%)	319 (97%)	9 (3%)	44	71
1	D	330/353 (94%)	309 (94%)	21 (6%)	17	33
1	E	329/353 (93%)	316 (96%)	13 (4%)	31	56
All	All	1315/1412 (93%)	1263 (96%)	52 (4%)	31	56

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	120	THR
1	A	180	SER
1	A	245	TRP
1	A	282	LEU
1	A	303	GLU
1	A	315	LEU
1	A	348	ILE
1	A	364	GLN
1	A	428	GLU
1	B	74	THR
1	B	214	VAL
1	B	245	TRP
1	B	262	LYS
1	B	282	LEU
1	B	287	LYS
1	B	364	GLN
1	B	373	SER
1	B	424	THR
1	D	48	VAL
1	D	60	GLN
1	D	67	THR
1	D	74	THR
1	D	152	GLU
1	D	178	ASP
1	D	197	LEU
1	D	214	VAL
1	D	221	SER
1	D	245	TRP
1	D	262	LYS
1	D	271	ASP
1	D	282	LEU
1	D	287	LYS
1	D	302	THR
1	D	315	LEU
1	D	340	THR
1	D	348	ILE
1	D	360	VAL
1	D	362	THR
1	D	424	THR
1	E	60	GLN
1	E	123	LYS
1	E	212	SER
1	E	217	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	235	SER
1	E	245	TRP
1	E	262	LYS
1	E	282	LEU
1	E	315	LEU
1	E	348	ILE
1	E	362	THR
1	E	424	THR
1	E	429	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 12 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	0VB	D	501	-	31,35,35	6.40	24 (77%)	43,49,49	3.82	24 (55%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	0VB	B	501	-	31,35,35	6.55	24 (77%)	43,49,49	4.09	25 (58%)
2	0VB	A	501	-	31,35,35	6.40	24 (77%)	43,49,49	3.91	25 (58%)
2	0VB	E	501	-	31,35,35	6.46	24 (77%)	43,49,49	3.75	25 (58%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	0VB	D	501	-	-	2/19/23/23	0/3/3/3
2	0VB	B	501	-	-	2/19/23/23	0/3/3/3
2	0VB	A	501	-	-	2/19/23/23	0/3/3/3
2	0VB	E	501	-	-	2/19/23/23	0/3/3/3

All (96) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	0VB	O29-C16	10.44	1.44	1.23
2	A	501	0VB	O29-C16	9.81	1.43	1.23
2	E	501	0VB	O29-C16	9.78	1.43	1.23
2	D	501	0VB	O29-C16	9.68	1.43	1.23
2	B	501	0VB	C05-C10	9.22	1.53	1.39
2	E	501	0VB	C05-C10	9.22	1.53	1.39
2	A	501	0VB	C05-C10	9.13	1.53	1.39
2	D	501	0VB	C05-C10	9.12	1.52	1.39
2	D	501	0VB	C11-C10	9.07	1.53	1.40
2	D	501	0VB	O30-C17	9.06	1.43	1.23
2	A	501	0VB	O30-C17	9.03	1.43	1.23
2	B	501	0VB	O30-C17	9.00	1.43	1.23
2	A	501	0VB	C11-C10	8.93	1.53	1.40
2	E	501	0VB	C11-C10	8.92	1.53	1.40
2	E	501	0VB	O30-C17	8.88	1.43	1.23
2	B	501	0VB	C14-N24	8.69	1.49	1.33
2	E	501	0VB	C06-C13	8.68	1.52	1.38
2	A	501	0VB	C14-N24	8.68	1.49	1.33
2	E	501	0VB	C14-N24	8.63	1.49	1.33
2	B	501	0VB	C06-C13	8.61	1.52	1.38
2	B	501	0VB	C11-C10	8.60	1.53	1.40
2	A	501	0VB	C03-C01	8.50	1.54	1.38
2	D	501	0VB	C06-C13	8.49	1.52	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	0VB	C14-N24	8.45	1.48	1.33
2	A	501	0VB	C06-C13	8.43	1.52	1.38
2	A	501	0VB	C11-C13	8.36	1.52	1.40
2	B	501	0VB	C03-C01	8.31	1.53	1.38
2	E	501	0VB	C03-C01	8.30	1.53	1.38
2	E	501	0VB	C06-C09	8.27	1.53	1.39
2	D	501	0VB	C03-C01	8.24	1.53	1.38
2	E	501	0VB	C05-C09	8.20	1.53	1.39
2	D	501	0VB	C11-C13	8.18	1.52	1.40
2	A	501	0VB	C05-C09	8.16	1.53	1.39
2	E	501	0VB	C11-C13	8.16	1.52	1.40
2	B	501	0VB	C11-C13	8.14	1.52	1.40
2	D	501	0VB	C05-C09	8.12	1.53	1.39
2	B	501	0VB	C06-C09	8.02	1.53	1.39
2	B	501	0VB	C05-C09	8.01	1.53	1.39
2	E	501	0VB	C08-C14	7.94	1.50	1.41
2	D	501	0VB	C06-C09	7.91	1.52	1.39
2	B	501	0VB	C08-C15	7.90	1.52	1.38
2	A	501	0VB	C06-C09	7.84	1.52	1.39
2	D	501	0VB	C03-C12	7.80	1.54	1.38
2	B	501	0VB	C18-N26	7.76	1.51	1.29
2	B	501	0VB	C04-C02	7.75	1.52	1.38
2	B	501	0VB	C03-C12	7.68	1.54	1.38
2	E	501	0VB	C03-C12	7.65	1.54	1.38
2	A	501	0VB	C03-C12	7.60	1.53	1.38
2	E	501	0VB	C08-C15	7.56	1.51	1.38
2	D	501	0VB	C08-C14	7.49	1.49	1.41
2	A	501	0VB	C04-C02	7.48	1.52	1.38
2	B	501	0VB	C04-C12	7.48	1.53	1.38
2	D	501	0VB	C04-C02	7.45	1.52	1.38
2	E	501	0VB	C04-C02	7.41	1.52	1.38
2	B	501	0VB	C08-C14	7.29	1.49	1.41
2	A	501	0VB	C04-C12	7.25	1.53	1.38
2	E	501	0VB	C04-C12	7.22	1.53	1.38
2	D	501	0VB	C08-C15	7.20	1.51	1.38
2	A	501	0VB	C08-C15	7.14	1.51	1.38
2	D	501	0VB	C04-C12	7.12	1.52	1.38
2	A	501	0VB	C08-C14	7.04	1.49	1.41
2	D	501	0VB	C01-C07	6.82	1.53	1.39
2	E	501	0VB	C01-C07	6.78	1.53	1.39
2	A	501	0VB	C18-N26	6.77	1.48	1.29
2	B	501	0VB	C16-N25	6.75	1.49	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	0VB	C01-C07	6.72	1.53	1.39
2	E	501	0VB	C17-N27	6.70	1.48	1.36
2	D	501	0VB	C18-N26	6.64	1.48	1.29
2	A	501	0VB	C17-N27	6.64	1.48	1.36
2	B	501	0VB	C17-N27	6.61	1.48	1.36
2	E	501	0VB	C18-N26	6.58	1.47	1.29
2	A	501	0VB	C01-C07	6.57	1.53	1.39
2	D	501	0VB	C17-N27	6.52	1.48	1.36
2	B	501	0VB	C02-C07	6.49	1.53	1.39
2	A	501	0VB	C02-C07	6.36	1.52	1.39
2	E	501	0VB	C02-C07	6.36	1.52	1.39
2	D	501	0VB	C02-C07	6.35	1.52	1.39
2	D	501	0VB	C16-N25	5.81	1.48	1.37
2	E	501	0VB	C16-N25	5.78	1.47	1.37
2	A	501	0VB	C16-N25	5.70	1.47	1.37
2	B	501	0VB	C15-S32	3.91	1.78	1.71
2	E	501	0VB	C15-S32	3.88	1.78	1.71
2	A	501	0VB	C15-S32	3.79	1.78	1.71
2	D	501	0VB	C15-S32	3.66	1.78	1.71
2	E	501	0VB	O31-C12	2.72	1.43	1.37
2	A	501	0VB	O31-C12	2.68	1.43	1.37
2	B	501	0VB	C07-C14	2.65	1.52	1.49
2	B	501	0VB	O31-C12	2.65	1.43	1.37
2	D	501	0VB	O31-C12	2.55	1.42	1.37
2	E	501	0VB	C11-N27	2.48	1.48	1.43
2	B	501	0VB	C11-N27	2.42	1.48	1.43
2	D	501	0VB	C07-C14	2.36	1.51	1.49
2	E	501	0VB	C07-C14	2.33	1.51	1.49
2	D	501	0VB	C11-N27	2.33	1.47	1.43
2	A	501	0VB	C07-C14	2.28	1.51	1.49
2	A	501	0VB	C11-N27	2.27	1.47	1.43

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	0VB	C21-C17-N27	10.73	130.72	114.98
2	A	501	0VB	C21-C17-N27	10.53	130.42	114.98
2	E	501	0VB	C21-C17-N27	10.43	130.29	114.98
2	D	501	0VB	C21-C17-N27	10.16	129.89	114.98
2	B	501	0VB	C23-N28-C18	7.77	132.31	123.08
2	A	501	0VB	C23-C09-C05	7.09	135.97	120.64
2	E	501	0VB	C23-C09-C05	7.02	135.82	120.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	0VB	C23-C09-C05	7.00	135.77	120.64
2	D	501	0VB	C23-C09-C05	6.85	135.44	120.64
2	B	501	0VB	C08-C16-N25	6.55	123.81	114.81
2	D	501	0VB	C08-C16-N25	6.47	123.70	114.81
2	A	501	0VB	C08-C16-N25	6.36	123.55	114.81
2	D	501	0VB	C23-N28-C18	6.31	130.58	123.08
2	B	501	0VB	O29-C16-C08	-6.22	111.59	120.95
2	A	501	0VB	C06-C13-CL1	-6.18	108.52	118.49
2	E	501	0VB	C08-C16-N25	6.16	123.28	114.81
2	D	501	0VB	O29-C16-C08	-6.15	111.68	120.95
2	E	501	0VB	C23-N28-C18	6.06	130.28	123.08
2	B	501	0VB	C22-O31-C12	6.05	130.64	117.51
2	B	501	0VB	O30-C17-N27	-6.01	115.14	123.04
2	A	501	0VB	C23-N28-C18	5.85	130.03	123.08
2	A	501	0VB	O29-C16-C08	-5.81	112.20	120.95
2	B	501	0VB	C06-C13-CL1	-5.76	109.19	118.49
2	A	501	0VB	C11-C13-CL1	5.72	125.83	119.27
2	B	501	0VB	C14-N24-S32	5.70	113.22	104.81
2	D	501	0VB	C15-C08-C14	5.70	115.11	104.65
2	A	501	0VB	O30-C17-N27	-5.69	115.56	123.04
2	E	501	0VB	C22-O31-C12	5.67	129.81	117.51
2	A	501	0VB	C15-C08-C14	5.59	114.91	104.65
2	D	501	0VB	C22-O31-C12	5.56	129.57	117.51
2	A	501	0VB	C22-O31-C12	5.53	129.51	117.51
2	D	501	0VB	O30-C17-N27	-5.35	116.00	123.04
2	B	501	0VB	C15-C08-C14	5.34	114.46	104.65
2	E	501	0VB	C15-C08-C14	5.31	114.39	104.65
2	E	501	0VB	C14-N24-S32	5.25	112.54	104.81
2	E	501	0VB	O30-C17-N27	-5.22	116.18	123.04
2	B	501	0VB	C13-C11-C10	-5.21	114.15	119.87
2	D	501	0VB	C06-C13-CL1	-5.19	110.11	118.49
2	D	501	0VB	C14-N24-S32	5.12	112.36	104.81
2	A	501	0VB	C23-C09-C06	-5.09	109.64	120.64
2	B	501	0VB	C08-C14-N24	-5.04	108.79	114.75
2	D	501	0VB	C08-C14-N24	-5.00	108.84	114.75
2	D	501	0VB	C23-C09-C06	-4.96	109.93	120.64
2	B	501	0VB	C11-C13-CL1	4.94	124.92	119.27
2	E	501	0VB	C23-C09-C06	-4.93	109.99	120.64
2	A	501	0VB	C13-C11-C10	-4.92	114.46	119.87
2	E	501	0VB	C06-C13-CL1	-4.92	110.54	118.49
2	D	501	0VB	C11-C13-CL1	4.90	124.89	119.27
2	E	501	0VB	O29-C16-C08	-4.86	113.64	120.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	501	0VB	C13-C11-C10	-4.79	114.61	119.87
2	A	501	0VB	C14-N24-S32	4.78	111.85	104.81
2	E	501	0VB	C08-C14-N24	-4.75	109.13	114.75
2	E	501	0VB	O30-C17-C21	-4.59	113.53	122.06
2	B	501	0VB	C23-C09-C06	-4.57	110.76	120.64
2	A	501	0VB	C08-C14-N24	-4.56	109.35	114.75
2	D	501	0VB	C13-C11-C10	-4.49	114.94	119.87
2	A	501	0VB	O30-C17-C21	-4.33	114.02	122.06
2	D	501	0VB	O30-C17-C21	-4.28	114.11	122.06
2	B	501	0VB	C09-C23-N28	4.27	122.20	113.05
2	B	501	0VB	O30-C17-C21	-4.27	114.14	122.06
2	B	501	0VB	C06-C09-C05	-4.17	113.26	118.98
2	E	501	0VB	C11-C13-CL1	3.83	123.66	119.27
2	E	501	0VB	C06-C09-C05	-3.78	113.79	118.98
2	B	501	0VB	C10-C05-C09	3.65	126.43	122.21
2	B	501	0VB	C02-C07-C14	3.65	126.38	120.61
2	A	501	0VB	C09-C23-N28	3.54	120.64	113.05
2	A	501	0VB	C06-C09-C05	-3.52	114.15	118.98
2	E	501	0VB	C10-C05-C09	3.41	126.16	122.21
2	D	501	0VB	C06-C09-C05	-3.38	114.34	118.98
2	A	501	0VB	C20-C15-S32	3.16	124.11	120.10
2	D	501	0VB	C02-C07-C14	3.12	125.55	120.61
2	B	501	0VB	C13-C11-N27	3.11	124.86	121.14
2	D	501	0VB	C20-C15-S32	3.11	124.04	120.10
2	A	501	0VB	C13-C11-N27	3.09	124.83	121.14
2	B	501	0VB	C06-C13-C11	3.08	125.88	121.81
2	A	501	0VB	C04-C02-C07	3.08	125.56	121.13
2	E	501	0VB	C04-C02-C07	3.06	125.55	121.13
2	A	501	0VB	C10-C05-C09	3.04	125.73	122.21
2	E	501	0VB	C02-C07-C14	3.03	125.40	120.61
2	E	501	0VB	C06-C13-C11	3.02	125.79	121.81
2	B	501	0VB	C04-C02-C07	2.96	125.40	121.13
2	A	501	0VB	C06-C13-C11	2.90	125.64	121.81
2	D	501	0VB	C04-C02-C07	2.83	125.20	121.13
2	D	501	0VB	C09-C23-N28	2.72	118.89	113.05
2	D	501	0VB	C10-C05-C09	2.71	125.34	122.21
2	E	501	0VB	C20-C15-S32	2.70	123.53	120.10
2	B	501	0VB	C20-C15-S32	2.53	123.31	120.10
2	D	501	0VB	C06-C13-C11	2.42	125.00	121.81
2	E	501	0VB	C14-C08-C16	2.41	131.77	127.08
2	A	501	0VB	C02-C07-C14	2.37	124.36	120.61
2	B	501	0VB	C14-C08-C16	2.34	131.65	127.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	0VB	C18-N25-C16	-2.22	121.31	125.58
2	E	501	0VB	C18-N25-C16	-2.19	121.36	125.58
2	B	501	0VB	C01-C03-C12	2.14	122.35	119.73
2	A	501	0VB	C01-C03-C12	2.13	122.33	119.73
2	E	501	0VB	C10-C11-N27	2.07	122.21	119.00
2	A	501	0VB	C18-N25-C16	-2.04	121.66	125.58
2	D	501	0VB	C14-C08-C16	2.03	131.05	127.08
2	E	501	0VB	C01-C03-C12	2.03	122.21	119.73

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	501	0VB	C01-C07-C14-N24
2	B	501	0VB	C01-C07-C14-N24
2	E	501	0VB	C01-C07-C14-N24
2	A	501	0VB	C01-C07-C14-N24
2	E	501	0VB	C02-C07-C14-N24
2	D	501	0VB	C02-C07-C14-N24
2	B	501	0VB	C02-C07-C14-N24
2	A	501	0VB	C02-C07-C14-N24

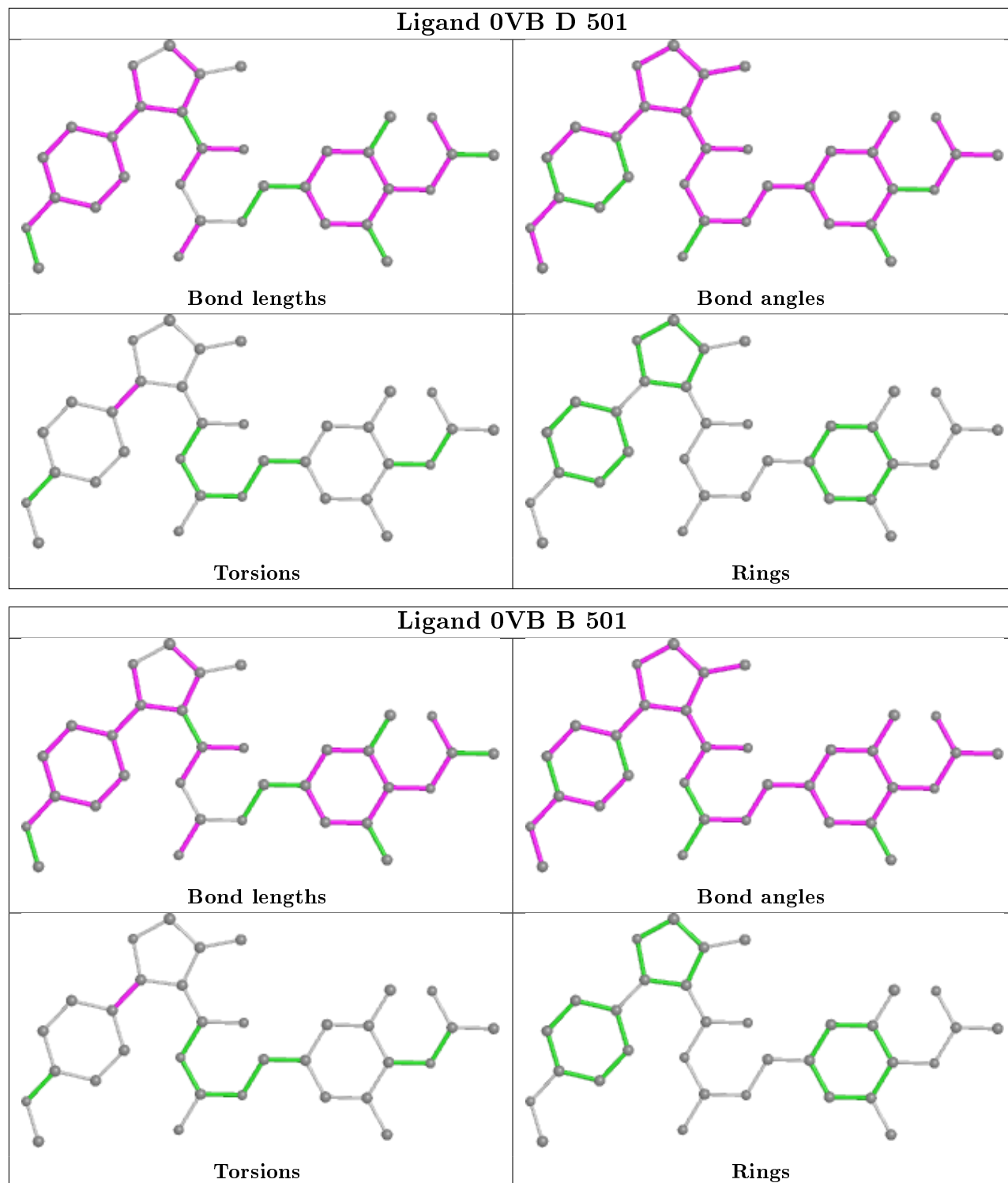
There are no ring outliers.

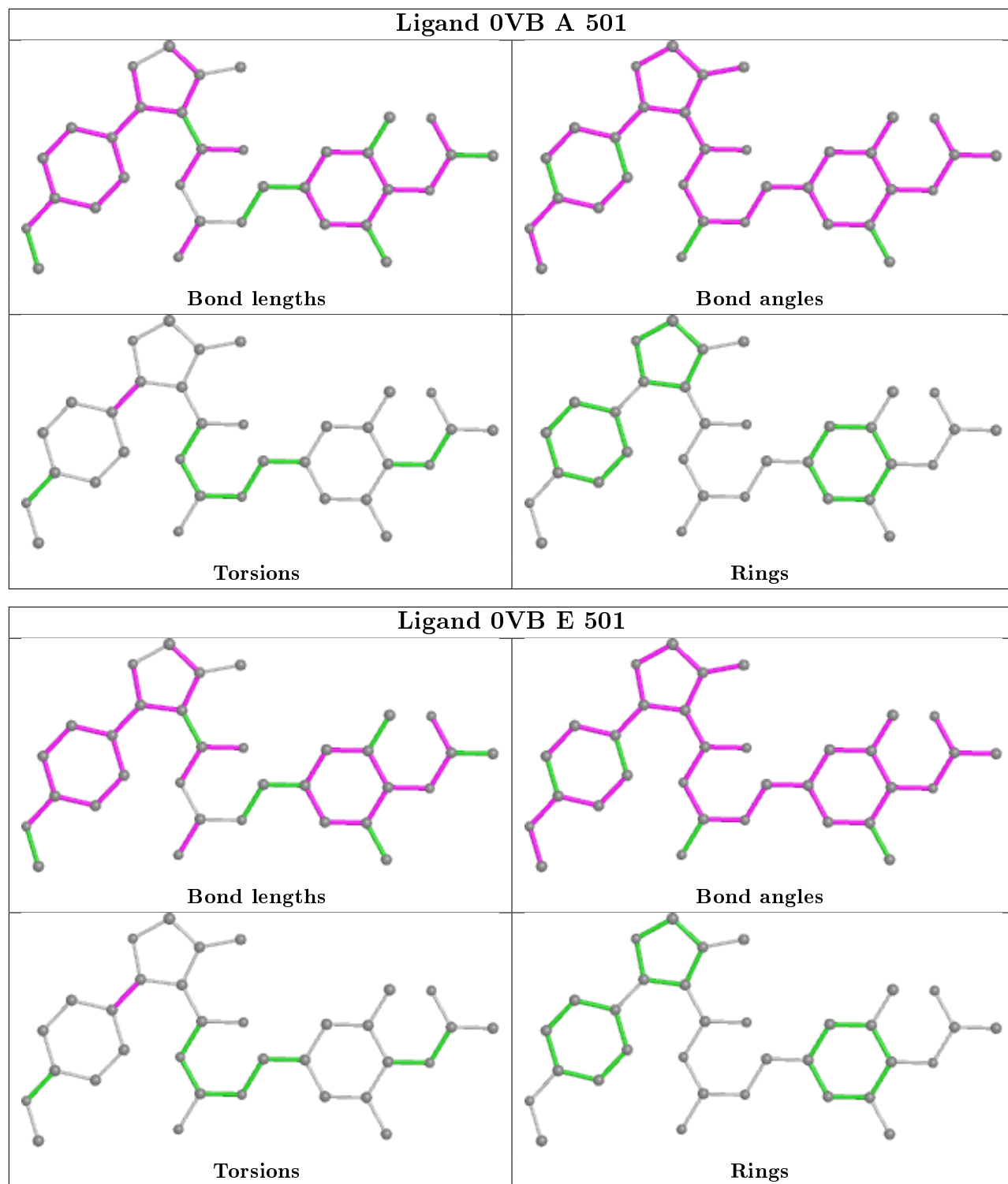
4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	0VB	2	0
2	B	501	0VB	3	0
2	A	501	0VB	4	0
2	E	501	0VB	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

equivalents in the CSD to analyse the geometry.





5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	387/412 (93%)	0.09	15 (3%) 39 42	18, 25, 37, 43	0
1	B	387/412 (93%)	0.05	12 (3%) 49 52	18, 25, 36, 40	0
1	D	387/412 (93%)	0.06	12 (3%) 49 52	18, 26, 38, 42	0
1	E	387/412 (93%)	0.07	10 (2%) 56 59	18, 25, 36, 40	0
All	All	1548/1648 (93%)	0.07	49 (3%) 47 51	18, 25, 37, 43	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	360	VAL	7.5
1	B	362	THR	7.2
1	A	360	VAL	5.9
1	E	362	THR	5.5
1	D	361	ALA	5.2
1	D	362	THR	5.1
1	A	362	THR	5.0
1	B	360	VAL	4.8
1	A	306	PRO	4.8
1	A	305	PHE	4.5
1	A	307	ASP	4.3
1	A	361	ALA	3.9
1	E	97	HIS	3.6
1	D	307	ASP	3.6
1	E	360	VAL	3.4
1	A	193	HIS	3.2
1	B	307	ASP	3.1
1	D	193	HIS	2.9
1	E	47	PHE	2.8
1	A	304	LYS	2.7
1	B	97	HIS	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	48	VAL	2.6
1	D	363	SER	2.5
1	B	306	PRO	2.5
1	A	47	PHE	2.5
1	E	304	LYS	2.5
1	A	229	HIS	2.5
1	B	270	TYR	2.4
1	B	301	SER	2.3
1	B	361	ALA	2.3
1	D	304	LYS	2.3
1	E	305	PHE	2.3
1	B	302	THR	2.3
1	B	48	VAL	2.3
1	A	301	SER	2.3
1	A	432	TYR	2.3
1	D	426	ASP	2.2
1	D	116	TYR	2.2
1	E	116	TYR	2.2
1	E	361	ALA	2.2
1	D	47	PHE	2.2
1	A	314	GLN	2.1
1	A	363	SER	2.1
1	B	426	ASP	2.1
1	D	359	ASP	2.1
1	D	305	PHE	2.0
1	A	429	ASP	2.0
1	E	229	HIS	2.0
1	B	359	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

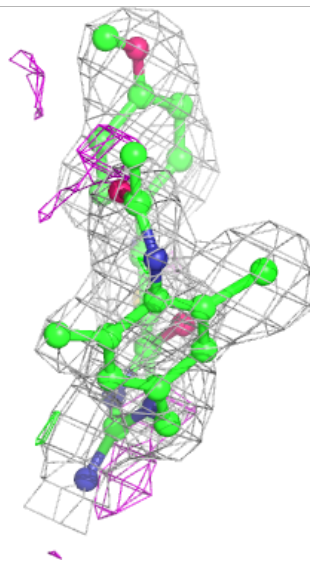
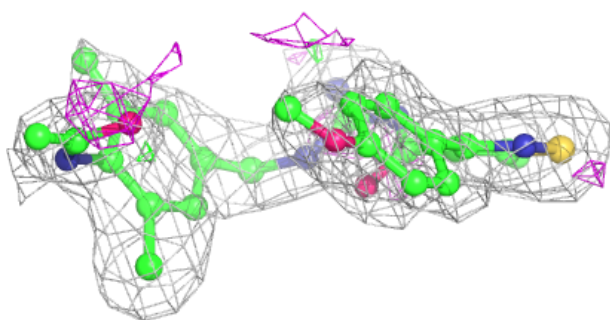
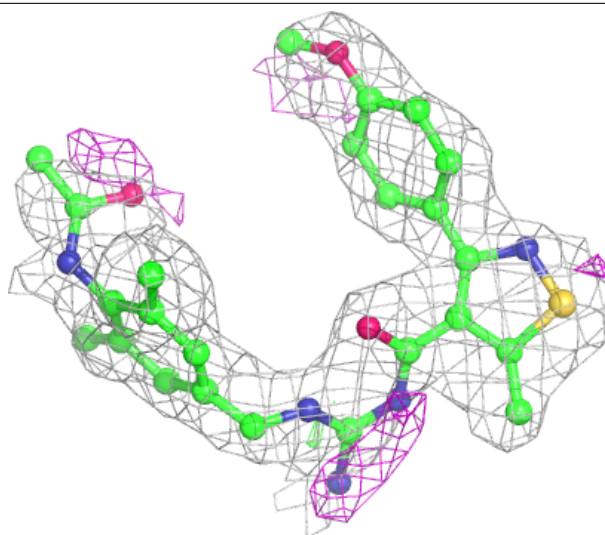
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	IOD	B	503	1/1	0.80	0.13	142,142,142,142	0
3	IOD	D	503	1/1	0.89	0.10	111,111,111,111	0
2	0VB	B	501	33/33	0.92	0.20	20,22,26,27	0
2	0VB	E	501	33/33	0.93	0.20	20,22,25,26	0
2	0VB	A	501	33/33	0.93	0.20	21,22,23,24	0
2	0VB	D	501	33/33	0.93	0.18	18,20,23,24	0
3	IOD	B	504	1/1	0.94	0.07	78,78,78,78	0
3	IOD	A	503	1/1	0.94	0.14	135,135,135,135	0
3	IOD	A	502	1/1	0.95	0.13	97,97,97,97	0
3	IOD	E	503	1/1	0.96	0.10	99,99,99,99	0
3	IOD	B	502	1/1	0.97	0.06	76,76,76,76	0
3	IOD	A	504	1/1	0.97	0.05	66,66,66,66	0
3	IOD	D	504	1/1	0.97	0.06	80,80,80,80	0
3	IOD	E	504	1/1	0.98	0.03	71,71,71,71	0
3	IOD	E	502	1/1	0.98	0.04	69,69,69,69	0
3	IOD	D	502	1/1	0.98	0.07	74,74,74,74	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

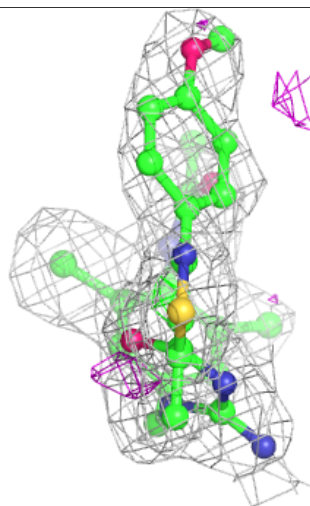
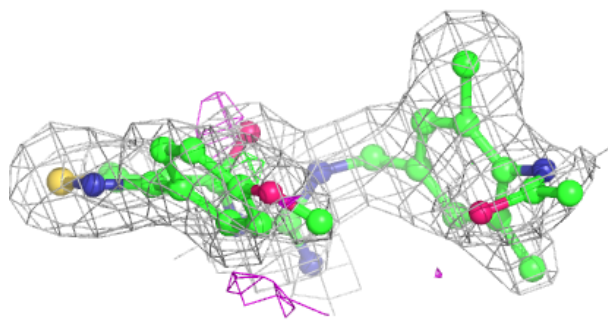
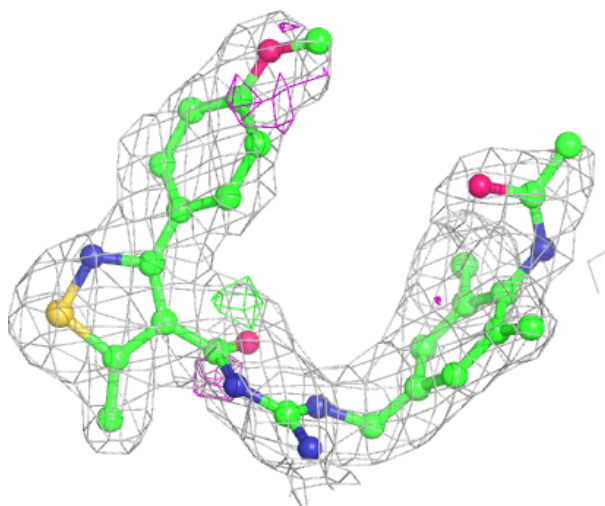
Electron density around 0VB B 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



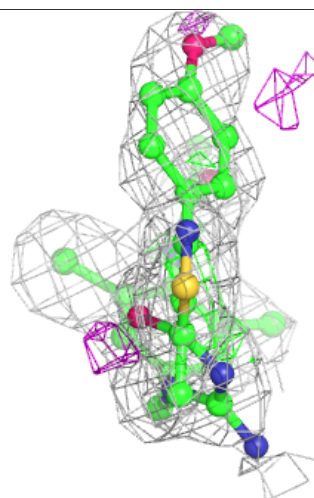
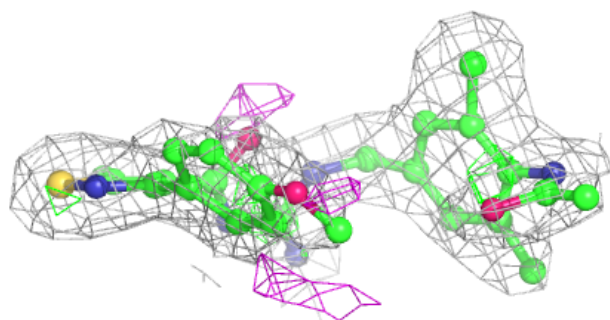
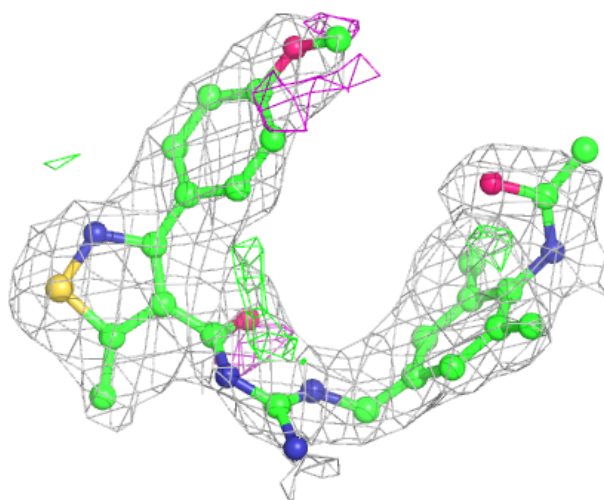
Electron density around 0VB E 501:

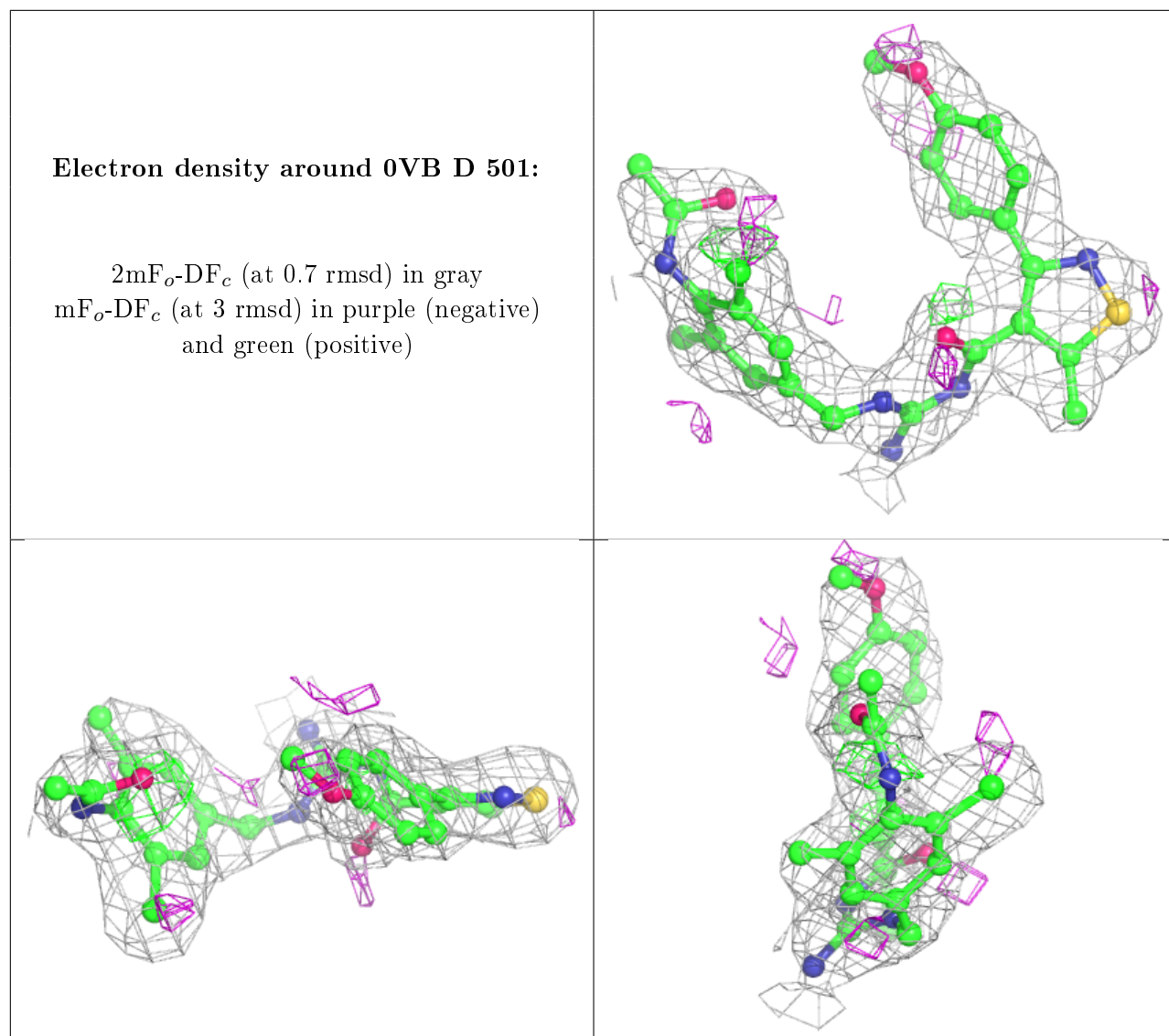
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 0VB A 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.